

# Influence of boundary conditions on level statistics and eigenstates at the metal insulator transition

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## Abstract

We investigate the influence of the boundary conditions on the scale invariant critical level statistics at the metal insulator transition of disordered three-dimensional orthogonal and two-dimensional unitary and symplectic tight-binding models. The distribution of the spacings between consecutive eigenvalues is calculated numerically and shown to be different for periodic and Dirichlet boundary conditions whereas the critical disorder remains unchanged. The peculiar correlations of the corresponding critical eigenstates leading to anomalous diffusion seem not to be affected by the change of the boundary conditions.

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## 1 Introduction and Model

The statistics of energy eigenvalues has proven to be a powerful tool to describe the localization-delocalization transition (LDT) in disordered electronic systems. For three-dimensional models, numerical work [1–6] and analytical investigations [7–11] have revealed a variety of new features and important relations that constitute the peculiar dynamics at the metal insulator transition. Also two-dimensional systems that exhibit a LDT were investigated numerically, e.g., electrons in a strong perpendicular magnetic field which show the quantum Hall effect (QHE) [12–14] or in the presence of spin-orbit interaction leading to a symplectic symmetry [15–17].

It has been suggested recently that the eigenvalue statistics directly at the critical point depend on the boundary conditions [18] and also on the shape of the sample [19] even in the limit of infinite system size. The so called critical statistics are scale independent and distinct from both the random matrix theory result which is appropriate for disordered systems with conducting electrons (extended states) and the Poisson law that describes the statistics of uncorrelated eigenvalues typically found for insulating (localized) states. The probability of eigenvalues being close

in energy is drastically reduced for extended states (level repulsion) while it is maximal for localized states due to the negligible overlap of the corresponding eigenstates.

The reported dependence of the critical level statistics on the boundary conditions [18] and on the sample shape [19] seems at first glance to be somewhat counter intuitive because in general for macroscopic samples one expects physical observables not to be sensitive to boundary effects. However, for mesoscopic systems it is known that the preserved phase coherence gives rise to various macroscopic quantum effects originating from, e.g., an applied Aharonov-Bohm flux which can be completely incorporated into the boundary conditions. It remains, however, to be seen whether or not the observed sensitivity of the level statistics with respect to changes of the boundary conditions will have an effect on measurable physical quantities. A related question is the possible influence of the boundary conditions on the critical wave functions which were shown to be multifractal objects [20–29]. The strong amplitude fluctuations of the eigenstates are responsible for anomalous diffusion which can be described by correlation functions characterized by an exponent  $\eta$  [30–32].

In this paper, we address the questions whether the influence on the boundary conditions is also present in 2d critical systems and if the eigenstates of the 3d Anderson model are affected too. Therefore, we present results of a numerical investigation of the critical eigenvalue statistics and the correlations of the corresponding eigenvectors. We consider standard tight binding Hamiltonians with diagonal disorder on a simple cubic lattice for 3d (Anderson model) and on square lattices for the 2d QHE [33] and the 2d symplectic model [34]. The disorder potentials  $\{\varepsilon_n\}$  are independent random numbers evenly distributed around zero. The width of this box distribution determines the disorder strength  $W$ . The Hamiltonian for the 3d orthogonal case (preserved time reversal symmetry) is given by

$$H = \sum_n \varepsilon_n c_n^\dagger c_n + \sum_{\langle m \neq n \rangle} V_{mn} c_m^\dagger c_n, \quad (1)$$

where  $c_n^\dagger, c_n$  are the creation and annihilation operators, respectively, and  $\{m, n\}$  denote the sites on the cubic lattice with lattice constant  $a$ . The transfer  $V_{mn} \equiv V = 1$  is restricted to nearest neighbors only and defines the unit of energy. For the 2d unitary system (broken time reversal symmetry) the Hamilton operator is the same (Eq. 1), except that  $\{m, n\}$  now represent the sites of a square lattice. Here, the magnetic field  $B$  is incorporated into the complex phase factors of the transfer terms,  $V_{mn} = V \exp(i2\pi e/h \int_{\mathbf{r}_m}^{\mathbf{r}_n} \mathbf{A}(\mathbf{r}) d\mathbf{r})$ , and the Landau gauge is chosen for the vector potential  $\mathbf{A} = (0, -B\mathbf{x}, 0)$ . The 2d symplectic model (broken spin-rotational invariance) is described by [34]

$$H = \sum_{m,\sigma} \varepsilon_m c_{m,\sigma}^\dagger c_{m,\sigma} + \sum_{\langle m \neq n \rangle, \sigma \sigma'} V(m, \sigma; n, \sigma') c_{m,\sigma}^\dagger c_{n,\sigma'}. \quad (2)$$

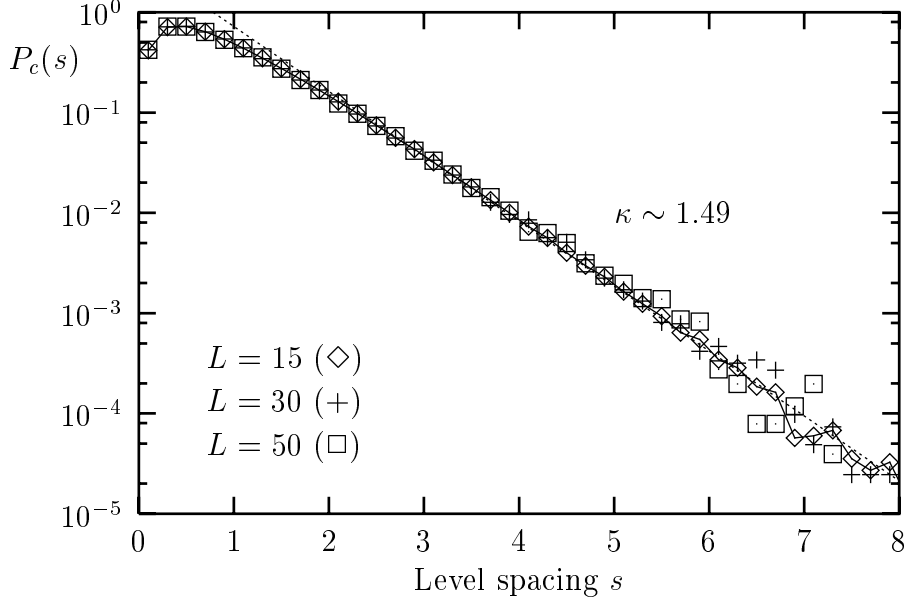


Fig. 1. Critical level spacing distribution,  $P_c(s)$ , for a 3d orthogonal system with Dirichlet boundary conditions (DBC).

The spin-orbit interaction strength  $S$  is defined as the ratio  $S = V_2/(V_1^2 + V_2^2)^{1/2}$ , where  $V_1$  and  $V_2$  are matrix elements of the  $2 \times 2$  complex transition matrices  $V(m, \sigma; n, \sigma')$  [34], which depend on the transfer-direction and on spin  $\sigma$ . In the following we choose the maximal value  $S = 0.5$  and define the unit of energy by  $V \equiv (V_1^2 + V_2^2)^{1/2} = 1$ . The eigenvalues are calculated using a Lanczos algorithm and care is taken to properly unfold the spectrum in order to distinguish local fluctuations of the eigenvalues from possible global changes in the density of states.

## 2 Results and Discussions

The nearest neighbor level spacing distribution,  $P_c(s)$ , of the 3d orthogonal system (Anderson model) is shown in Fig. 1 for Dirichlet boundary conditions (DBC). As usual, the spacings  $s = |E_{i+1} - E_i|/\Delta$  of successive eigenenergies  $\{E_i\}$  are divided by the mean level spacing  $\Delta$ . The curves are obtained at the critical disorder  $W_c = 16.4 V$  for different system sizes  $L/a = 15, 30$ , and  $50$ , which is more than a factor of 2 larger than in [18], but still no size dependence can be observed. The corresponding values of the second moment,  $J_c \equiv \langle s^2 \rangle = \int_0^\infty s^2 P_c(s) ds$ , are calculated to be  $J_c(L/a = 15) = 1.608$ ,  $J_c(L/a = 30) = 1.617$ , and  $J_c(L/a = 50) = 1.616$ , which are in accord with those of Ref. [18]. While for small  $s$ ,  $P_c(s) \sim s$ , as expected from RMT, the large- $s$  behavior is well approximated by a simple exponential decay,  $P_c(s) \sim \exp(-\kappa s)$ , with  $\kappa_{\text{DBC}} \approx 1.49$  which is significantly smaller than the result for periodic boundary conditions (PBC),  $\kappa_{\text{PBC}} \approx 1.9$  [4,5].

A correlation function of the corresponding critical eigenfunctions  $\psi_E(x)$  is shown

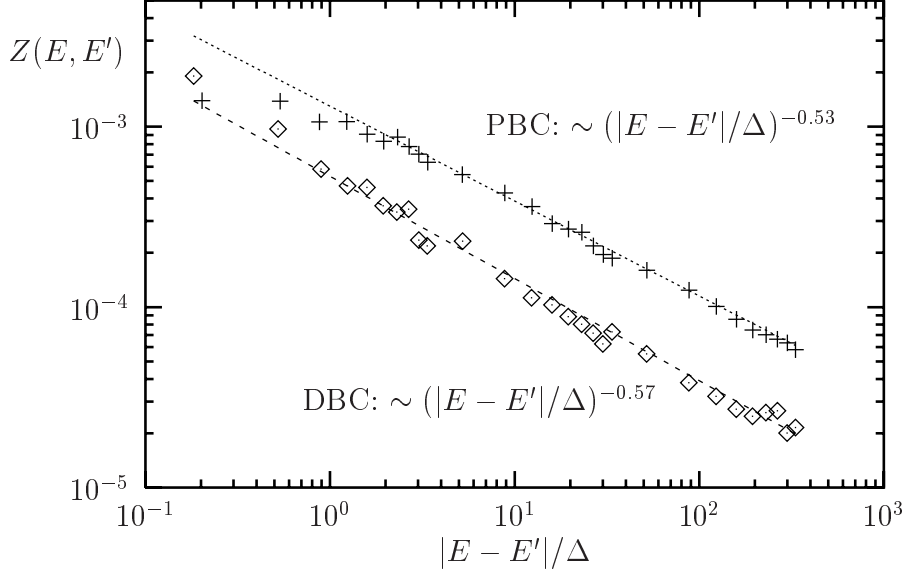


Fig. 2. Critical eigenfunction correlations for a 3d system of size  $L = 40a$  with Dirichlet (DBC) and periodic boundary conditions (PBC).

in Fig. 2 for a system of linear size  $L = 40a$  and different boundary conditions. As in Ref. [32] we compute the function

$$Z(E, E') = \int_0^\infty |\psi_E(x)|^2 |\psi_{E'}(x)|^2 d^d x \sim \left( \frac{|E - E'|}{\Delta} \right)^{-\mu} \quad (3)$$

from which the exponent  $\mu = \eta/d$  can be extracted.  $\eta$  is related to the fractal correlation dimension  $D(2) = d - \eta$  [27]. In the logarithmic plot the power law behavior  $Z(E, E') \sim (|E - E'|/\Delta)^{-\mu}$  becomes apparent. We find two exponents  $\mu_{PBC} = 0.53 \pm 0.1$  and  $\mu_{DBC} = 0.57 \pm 0.1$  which are indistinguishable within the uncertainty of our data.

A similar behavior as in 3d is observed for the level statistics of the two-dimensional system with spin-orbit interaction that shows also a complete metal insulator transition at a critical disorder  $W_c \simeq 6.0 V$  [17]. Within numerical uncertainty the critical  $P_c(s)$  for DBC is scale independent and distinct from the one with PBC (see Fig. 3). This manifests itself in the different decay constants  $\kappa_{PBC} = 3.8 \pm 0.2$  and  $\kappa_{DBC} = 2.8 \pm 0.2$ . The values for the second moments of the critical symplectic distributions are  $J_c^{PBC} = 1.142$  and  $J_c^{DBC} = 1.254$ . The attempts to look for another critical disorder at which  $P_c(s)$  for DBC coincides with the level spacing distribution for PBC at  $W_c \simeq 6.0 V$ , as suggested in Ref. [35] for the QHE system, ended without any result.

The situation for the 2d QHE-system is similar, however, due to the incomplete metal insulator transition the case is more complicated. In a QHE-system all states are localized with a localization length diverging at singular energies  $E_n$ . At these

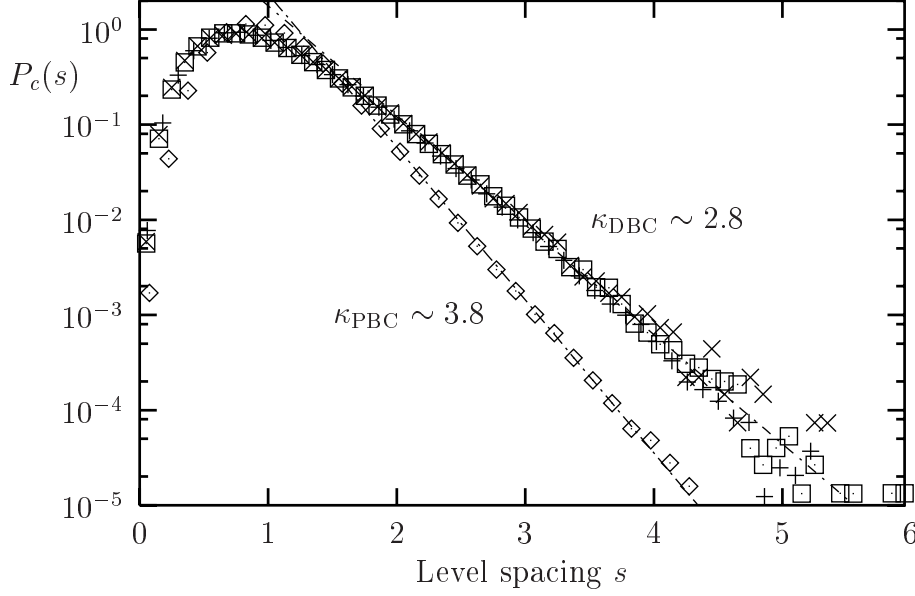


Fig. 3. Critical level spacing distribution of 2d symplectic systems with PBC of size  $L = 20a$  ( $\diamond$ ), and with DBC of size  $L = 40a$  (+),  $L = 80a$  ( $\square$ ), and  $L = 120a$  ( $\times$ ). The large- $s$  behavior is well fitted by  $P_c(s) \sim \exp(-\kappa s)$ .

critical points the eigenstates are multifractal [22,26–28] and a normal extended phase is absent. The application of Dirichlet boundary conditions introduces edge states that extend along the sample boundaries which seems to cause a certain shift of the critical energies  $E_n$  [35]. The question remains, whether the small differences that we found between the two distributions will show up also in the limit of infinite system size.

In conclusion, we have shown that the scale independent critical energy level statistics are influenced by the boundary conditions in 2d and 3d systems. For the 3d Anderson model, the correlations of the corresponding eigenstates seem not to be affected by a change of the boundary conditions, at least within the uncertainty of our calculations.

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